CHAPTER II

THE INFINITE AND THE SEMI-INFINITE CHAINS

In this chapter,the infinite linear and the semi-infinite linear chains have been reviewed form the works of E.N. Martinez[1], L. Brillouin[2], and N.W. Ashcroft and N.D. Mermin[3].

The Infinite Linear Chain

We have considered and reviewed in two cases,the first one : the infinite monatomic linear chain and the last one : the infinite diatomic linear chain, as follows.

2.1 The Infinite Monatomic Linear Chain[4,5]

It is a string of equal masses,m, each one connected to its neighbors on the both sides by the identical massless spring of constant C. A mass m will have its neighbors a distance d. This is shown in Fig. 2.1.1

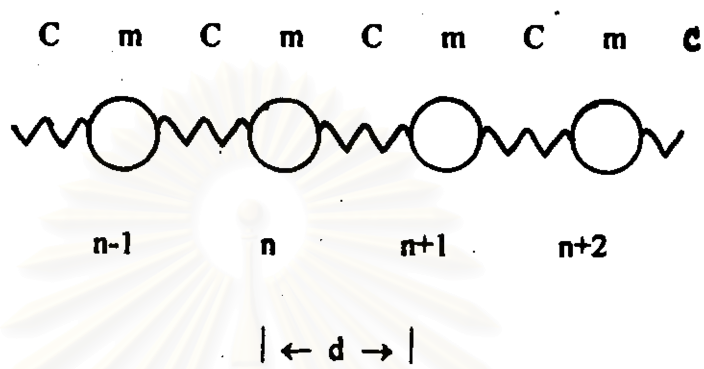

Fig. 2.1.1 The Infinite Monatomic Linear Chain

In this thesis, we have discussed the longitudinal displacement and the interactions have been taken place between the first nearest neighbors only.

The displacement of the n th mass m from its equilibrium position along the line that connects it to its neighbors is called as u_n.

The Hamitonian for the chain is

$$H = (1/2m)\sum_{n=-\infty}^{\infty} P_n^2 + (C/2)\sum_{n=-\infty}^{\infty}(u_{n+1} - u_n)^2 , \qquad (2.1.1)$$

where the definition of the linear momentum of mass is

$$m\dot{u}_n = P_n \quad , \tag{2.1.2}$$

and the equation of motion for n th mass is*

$$m\ddot{u} = C(u_{n+1} - u_n) + C(u_{n-1} - u_n) \quad . \tag{2.1.3}$$

2.2 <u>The Infinite Diatomic Linear Chain[2,3]</u>

The infinite diatomic linear chain is a string of difference masses ,m_1 and m_2, connected to each other by spring of constant ,C_1 and C_2. A given mass m_1 will have its right-hand neighbor a distance d_1 and its left-hand neighbor a distance d_2 on the other side. This is shown in Fig. 2.2.1

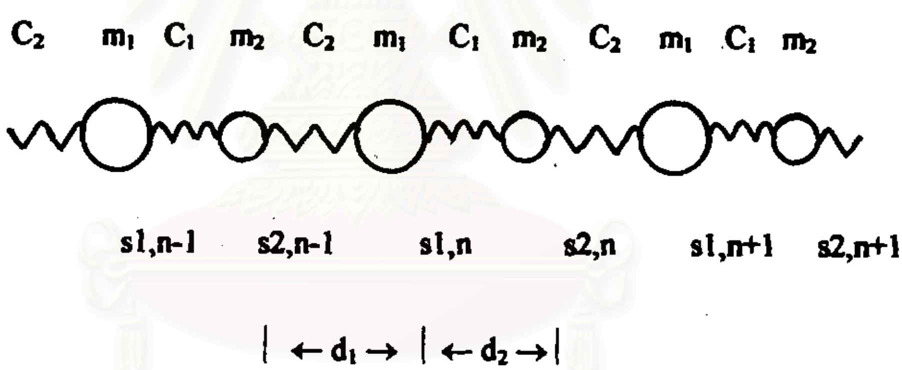

Fig. 2.2.1 The Infinite Diatomic Linear Chain

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*See APPENDIX A .

The displacement of the s1,n th mass m_1 from its equilibrium position along the line that connects it to its neighbors is called as $u_{s1,n}$. Similarly, The displacement of the s2,n th mass m_2 is called as $u_{s2,n}$. The indices s1,n and s2,n are numbers that count the masses m_1 and m_2 , respectively.

The Hamitonian for the chain is

$$H = (1/2m_1)\sum_{n=-\infty}^{\infty} P_{s1,n}^2 + (C_1/2)\sum_{n=-\infty}^{\infty}(u_{s2,n} - u_{s1,n})^2 + (1/2m_2)\sum_{n=-\infty}^{\infty} P_{s2,n}^2 + (C_2/2)\sum_{n=-\infty}^{\infty}(u_{s1,n+1} - u_{s2,n})^2 \quad , \qquad (2.2.1)$$

where the definition of the linear momentum of each mass are

$$m_1 \dot{u}_{s1,n} = P_{s1,n} \quad , \qquad (2.2.2a)$$

$$m_2 \dot{u}_{s2,n} = P_{s2,n} \quad , \qquad (2.2.2b)$$

and the equations of motion for n th mass m_1 and m_2 are*

$$m_1 \ddot{u}_{s1,n} = C_1(u_{s2,n} - u_{s1,n}) + C_2(u_{s2,n-1} - u_{s1,n}) \quad , \qquad (2.2.3a)$$

$$m_2 \ddot{u}_{s2,n} = C_1(u_{s1,n} - u_{s2,n}) + C_2(u_{s1,n+1} - u_{s2,n}) \quad , \qquad (2.2.3b)$$

*See APPENDIX A.

The Semi-Infinite Linear Chain

Consider in two cases: the semi-infinite monatomic chain and the semi-infinite diatomic chain.

2.3 The Semi-Infinite Monatomic Linear Chain[1]

It is a string of equal masses,m, each one is connected to each other by identical massless spring of constant C; one side is the end and the other side extends without the end. This is shown in Fig. 2.3.1

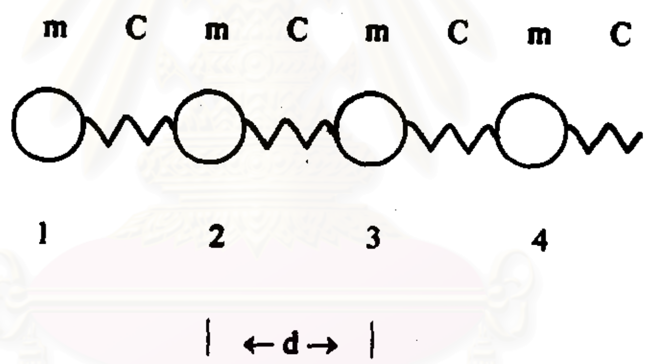

Fig. 2.3.1 The Semi-Infinite Monatomic Linear Chain

The Hamitonian for this semi-infinite monatomic chain is

$$H = (1/2m)\sum_{n=1}^{\infty} P_n^2 + (C/2)\sum_{n=1}^{\infty} (u_{n+1} - u_n)^2 . \qquad (2.3.1)$$

Then the equation of motion for the first mass is*

$$m\ddot{u}_1 = C(u_2 - u_1) \quad , \qquad (2.3.2)$$

while the equations of motion for the other mass is

$$m\ddot{u}_n = C(u_{n+1} - u_n) + C(u_{n-1} - u_n) \quad , \qquad (2.3.3)$$

where n is integer.

2.4 The Semi-Infinite Diatomic Linear Chain

The semi-infinite diatomic chain is a linear chain of difference masses, m_1 and m_2, are connected to each other by spring constants, C_1 and C_2; where one side is the end and the other side extends without the end. This is shown in Fig. 2.4.1

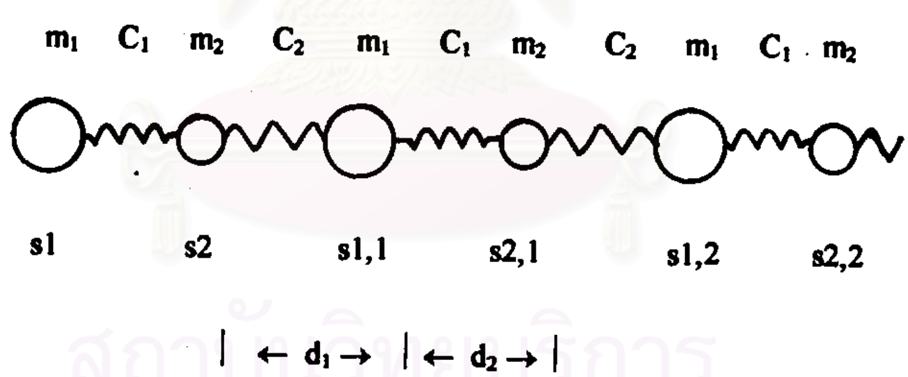

Fig. 2.4.1 The Semi-Infinite Diatomic Linear Chain

*See APPENDIX B.

The displacement of the s1,n th mass m_1 is called as $u_{s1,n}$. Similarly, the displacement of the s2,n th mass m_2 is called as $u_{s2,n}$.

The Hamitonian for the chain is

$$H = (1/2m_1)\sum_{n=0}^{\infty} P_{s1,n}^2 + (C_1/2)\sum_{n=0}^{\infty}(u_{s2,n} - u_{s1,n})^2 + (1/2m_2)\sum_{n=0}^{\infty} P_{s2,n}^2 + (C_2/2)\sum_{n=0}^{\infty}(u_{s1,n+1} - u_{s2,n})^2 \quad (2.4.1)$$

The equation of motion for the first mass (s1) is*

$$m_1 \ddot{u}_{s1} = C_1 (u_{s2} - u_{s1}) \quad , \quad (2.4.2a)$$

whereas the equations of motion for the other masses are

$$m_1 \ddot{u}_{s1,n} = C_1 (u_{s2,n} - u_{s1,n}) + C_2(u_{s2,n-1} - u_{s1,n}) \; ; n \geq 1 \quad , \quad (2.4.2b)$$

$$m_2 \ddot{u}_{s2,n} = C_1 (u_{s1,n} - u_{s2,n}) + C_2(u_{s1,n+1} - u_{s2,n}) \; ; \; n \geq 0 \quad . \quad (2.4.2c)$$

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*See APPENDIX B.